

Supplementary Table 1. Crystallographic data processing and refinement.

mutant	N2D	K3N	K21Q	L27D	R30Q	K31Q	L35S	P38G	K45S	K65Q	R88Q	K112Q	K120S
space group	P4 ₂ ,2 ₁	P4 ₂ ,2 ₁	P4 ₂ ,2 ₁	P4 ₂ ,2 ₁	P2 ₂ ,2 ₁	P4 ₂ ,2 ₁	P4 ₂ ,2 ₁	P2 ₂ ,2 ₁	C2	P4 ₃	P4 ₂ ,2 ₁	P4 ₂ ,2 ₁	P4 ₂ ,2 ₁
unit cell dimensions (Å, Å, Å, °, °, °)	58.26 58.26 101.72 90 90 90	64.5 64.5 101.2 90 90 90	57.96 57.96 101.24 90 90 90	64.88 64.88 100.92 90 90 90	58.59 75.96 100.63 90 90 90	58.24 58.24 102.19 90 90 90	65.83 65.83 101.32 90 90 90	55.54 65.49 82.23 90 90 90	120.13 63.61 94.47 90 130.1 90	83.03 83.03 77.90 90 90 90	64.88 64.88 264.35 90 90 90	65.71 65.71 101.19 90 90 90	63.68 63.68 101.4 90 90 90
resolution range (Å)	30-1.65 (1.70-1.65)	20-2-70 (2.77-2.70)	30-2.30 (2.36-2.30)	30-2.31 (2.37-2.31)	25-3.0 (3.08-3.00)	40-1.80 (1.85-1.80)	25-2.00 (2.05-2.00)	20-1.80 (1.85-1.80)	20-2.20 (2.26-2.20)	20-1.20 (1.23-1.20)	40-1.80 (1.85-1.80)	25-1.80 (1.85-1.80)	40-2.90 (2.98-2.90)
completeness (%)	97.4 (78.9)	99.5 (100)	99.2 (97.6)	98.9 (94.6)	98.4 (95.5)	98.7 (99.8)	98.2 (99.8)	90.9 (58.4)	88.0 (49.2)	93.9 (63.2)	99.4 (96.8)	99.4 (95.6)	99.6 (97.4)
$\langle 1/\sigma \rangle$	15.2 (1.5)	14.5 (3.1)	11.1 (2.2)	8.0 (0.9)	9.0 (1.2)	19.0 (2.5)	19.8 (1.7)	21.8 (2.2)	11.0 (1.6)	19.5 (1.4)	19.8 (2.0)	30.2 (2.0)	10.5 (1.8)
redundancy	4.7 (2.0)	10.7 (11.2)	5.1 (4.7)	7.9 (4.7)	4.7 (4.6)	9.5 (9.2)	12.3 (9.7)	5.5 (3.7)	3.4 (2.8)	5.1 (2.1)		11.8 (11.2)	7.2 (7.3)
R _{sym} (%)	8.0 (54.1)	17.3 (80.0)	13.8 (75.5)	21.7 (197.1)	12.6 (168.0)	11.1 (92.6)	10.0 (149.2)	4.9 (57.6)	7.8 (62.3)	4.1 (66.1)	7.9 (77.3)	6.1 (126.7)	13.3 (106.5)
completeness after anisotropic truncation				81.5	84.7		86.3						
R _{work} (%)	14.6	21.2	18.8	18.8	25.4	14.5	17.0	16.7	19.4	13.1	15.9	17.8	21.0
R _{free} (%)	18.8	25.0	22.4	24.5	28.9	18.9	21.3	22.5	25.2	15.4	19.9	20.3	25.7
RMSD bond length (Å)	0.009	0.002	0.003	0.003	0.003	0.008	0.012	0.012	0.004	0.010	0.010	0.012	0.003
RMSD bond angle (°)	1.1	0.5	0.6	0.5	0.6	1.0	1.0	1.2	0.8	1.1	1.1	1.4	0.5
Ramachandran favoured (%)	99.3	99.2	98.5	98.5	93.9	100	98.6	96.5	98.0	99.2	100	100	96.2
Ramachandran outliers (%)	0	0	0	0	0.4	0	0	0.4	0	0	0	0	0
Molprobit score, percentile	1.15, 99th	1.31, 100th	0.99, 100th	0.67 (100th)	2.03 (99th)	1.17 (99th)	1.14, 100th	1.62, 89th	1.82 (93rd)	1.41 (81st)	1.45 (96th)	1.78 (80th)	1.68 (100th)
PDB entry	6xu5	6xu9	6xua	6xuw	6sts	6xvq	6xvr	6xvs	4a1h	4a1y	6xvy	4a8z	6xw9